Package 'iSTATS'

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Type Package

Title A Graphical Interface to Perform STOCSY Analyses on NMR Data

Version 1.7

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Description Launches a 'shiny' based application for Nuclear Magnetic Resonance (NMR)data importation and Statistical TOtal Correlation SpectroscopY (STOCSY) analyses in a full interactive approach. The theoretical background and applications of STOCSY method could be found at Cloarec, O., Dumas, M. E., Craig, A., Barton, R. H., Trygg, J., Hudson, J., Blancher, C., Gauguier, D., Lindon, J. C., Holmes, E. & Nicholson, J. (2005) <doi:10.1021/ac048630x>.

Depends R(>= 3.6), shinyBS(>= 0.61), shinyWidgets(>= 0.4.3)

Imports Cairo(>= 1.5), ggplot2(>= 3.0.0), gtools(>= 3.8.1), shiny(>= 1.0.2), plotly, rstudioapi, data.table, readr

BugReports https://github.com/vitor-mendes-iq/iSTATS

Encoding UTF-8

LazyData true

RoxygenNote 7.1.1

NeedsCompilation no

License GPL (>= 3)

Repository CRAN

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Contents

CS_values_real *Matrix of NMR chemical shifts*

Description

A matrix containing all chemical shifts of NMR data milk samples

Usage

```
CS_values_real
```

Format

A matrix with 11 rows and 32778 variables:

file_names *A list of sample names*

Description

A list of sample names

Usage

```
file_names
```

Format

A list of string with sample names

iSTATS *A Graphical Interface to Perform STOCSY analyses on NMR Data*

Description

Statistical TOtal Correlation SpectroscopY (STOCSY) is a method developed to analyze 1D Nuclear Magnetic Resonance (NMR) data, with many applications in metabolomic science, as to help the identification of molecules in complex mixture. Although STOCSY is promising method, its use requires some programming language skills. To overcome this challenge we developed the interactive STATistical Spectroscopy (iSTATS) package, based on 'shiny', in which it is possible to perform STOCSY analyses in a full interactive way, from 1D NMR matrix construction to select specifical regions to apply STOCSY methods more accurately.

Usage

```
iSTATS()
```

Examples

```
if(interactive()){iSTATS::iSTATS()}
```

NMRData *Matrix of NMR intensities*

Description

A matrix containing the intensities of NMR data milk samples

Usage

```
NMRData
```

Format

A matrix with 11 rows and 32778 variables:

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